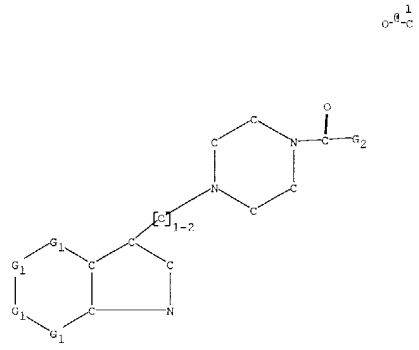
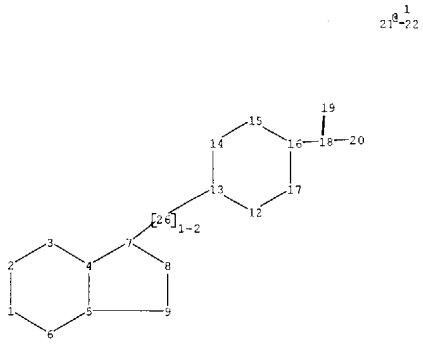
C:\Program Files\Stnexp\Queries\10038306.str

Updated for 10/630278
(from earlier parent)





chain nodes :
18 19 20 21 22 26
ring nodes :
1 2 3 4 5 6 7 8 9 12 13 14 15 16 17
chain bonds :
7-26 13-26 16-18 18-19 18-20 21-22
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-9 7-8 8-9 12-13 12-17 13-14 14-15 15-16
16-17
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-9 7-8 7-26 8-9 12-13 12-17 13-14 13-26 14-15
15-16 16-17 16-18 18-19 18-20 21-22
isolated ring systems :
containing 1 : 12 :

G1:C,N

G2:Cy,[*1]

Connectivity :
26:2 M minimum RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 12:Atom 13:Atom
14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS
26:CLASS

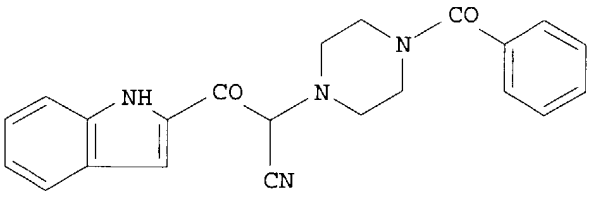
10/630278

```
=> s l6
SAMPLE SEARCH INITIATED 19:44:08 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     178 TO ITERATE

100.0% PROCESSED     178 ITERATIONS                                  0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          2760 TO     4360
PROJECTED ANSWERS:                0 TO        0

L7             0 SEA SSS SAM L6

=> s l6 sss full
FULL SEARCH INITIATED 19:44:18 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    3272 TO ITERATE

100.0% PROCESSED    3272 ITERATIONS                                  2 ANSWERS
SEARCH TIME: 00.00.01

L8             2 SEA SSS FUL L6

=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   155.84     331.60

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00      -1.39

FILE 'CAPLUS' ENTERED AT 19:44:37 ON 17 APR 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)


Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available
for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.
The CA Lexicon is the copyrighted intellectual property of the
American Chemical Society and is provided to assist you in searching
databases on STN.  Any dissemination, distribution, copying, or storing
of this information, without the prior written consent of CAS, is
strictly prohibited.

FILE COVERS 1907 - 17 Apr 2004  VOL 140 ISS 17
FILE LAST UPDATED: 16 Apr 2004  (20040416/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> s l8
L9             2 L8

=> d l9 1-2 bib abs hitstr
```

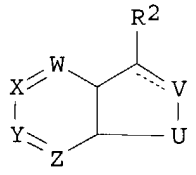
L9 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:832569 CAPLUS
DN 137:337880
TI Preparation of indole, azaindole, and related heterocyclic piperazinecarboxamides for treatment of AIDS
IN Wang, Tao; Wallace, Owen B.; Meanwell, Nicholas A.; Zhang, Zhongxing; Bender, John A.; Kadow, John F.; Yeung, Kap-Sun
PA Bristol-Myers Squibb Company, USA
SO PCT Int. Appl., 111 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002085301	A2	20021031	WO 2002-US12856	20020423
	WO 2002085301	A3	20030227		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2003096825	A1	20030522	US 2002-127256	20020422
	EP 1381366	A2	20040121	EP 2002-764315	20020423
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
PRAI	US 2001-286347P	P	20010425		
	WO 2002-US12856	W	20020423		

OS MARPAT 137:337880
GI



I



II

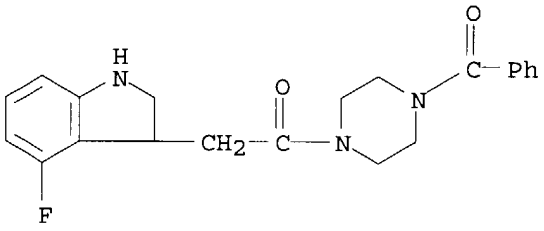
AB This invention provides indole, azaindole, and related heterocyclic piperazinecarboxamides Q(C(O))m(CR8R8')n(C(O))pTC(O)A (1; variables defined below; e.g. N-(benzoyl)-N'-[2-(indol-2-yl)-2-oxo-1-cyanoethyl]piperazine (shown as I)) having drug and bio-affecting properties, their pharmaceutical compns. and method of use. These compds. possess unique antiviral activity, whether used alone or in combination with other antivirals, antiinfectives, immunomodulators or HIV entry

inhibitors. More particularly, the present invention relates to the treatment of HIV and AIDS. EC50 ranges against HIV-1 are given for about 30 of the claimed compds.; for example, N-(benzoyl)-N'-[2-(6-methoxyindol-2-yl)-2-oxo-1-cyanoethyl]-3-methylpiperazine has an EC50 <1μM. Although the methods of preparation are not claimed, 32 example prepns. of 1 and 6 example prepns. of intermediates are included. In 1: Q is shown as II (dotted line may be a bond); A is C1-6alkoxy, C1-6alkyl, C3-7cycloalkyl, Ph, and heteroaryl; T is piperazine-1,4-diyl; U is NR7, O, or S; V is C(H)kR1, O or N(R7)k; W is CR3 or NR10; X is CR4 or NR10; Y is CR5 or NR10; Z is CR6 or NR10; k is 0 or 1; m, n, and p are 0-2 provided that the sum of m, n, and p must equal 1 or 2; R8 and R8 are H, hydroxy, C1-6alkyl, C1-6alkoxy, cyano, and fluoro, or R8 and R8' taken together form :O, :S, :NOR9, or :NH; other variables and provisos are given in the claims.

IT **474011-86-4P**, 1-(Benzoyl)-4-[(4-fluoroindolin-3-yl)acetyl]piperazine
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of indole, azaindole, and related heterocyclic piperazinecarboxamides for treatment of AIDS)

RN 474011-86-4 CAPLUS

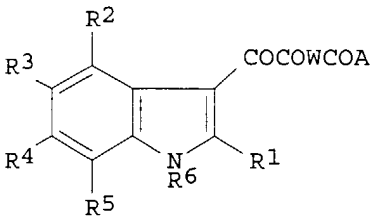
CN Piperazine, 1-benzoyl-4-[(4-fluoro-2,3-dihydro-1H-indol-3-yl)acetyl]-(9CI) (CA INDEX NAME)



L9 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:51452 CAPLUS
DN 136:118470
TI Preparation of substituted indoleoxoacetylpiperazines with antiviral activity against HIV-1
IN Wallace, Owen B.; Wang, Tao; Yeung, Kap-Sun; Pearce, Bradley C.; Meanwell, Nicholas A.; Qiu, Zhilei; Fang, Haiquan; Xue, Qiufen May; Yin, Zhiwei
PA Bristol-Myers Squibb Company, USA
SO PCT Int. Appl., 277 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002004440	A1	20020117	WO 2001-US20300	20010626
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1299382	A1	20030409	EP 2001-946715	20010626
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	JP 2004502768	T2	20040129	JP 2002-509305	20010626
PRAI	US 2000-217444P	P	20000710		
	US 2001-265978P	P	20010202		
	WO 2001-US20300	W	20010626		

OS MARPAT 136:118470
GI



I

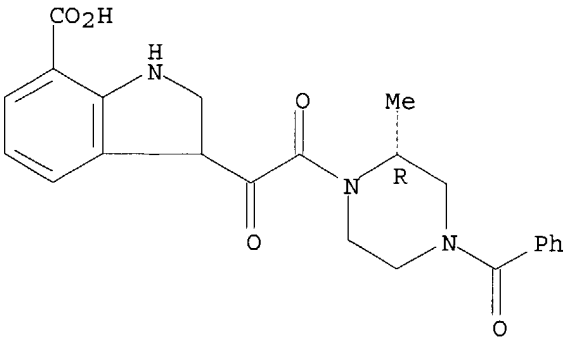
AB Indoleoxoacetylpiperazines I [A = (un)substituted alkoxy, aryl, heteroaryl; W = (un)substituted piperazino; R1 = H; R2-R5 = H, halogen, CN, NO2, (un)substituted NH2, OH, (un)substituted alkyl, cycloalkyl, alkoxy, CO2H, acyl, carbamoyl, amidino, aryl, heteroaryl, heterocyclic; R6 = H, alkyl] and their 2,3-dihydroindole analogs were prepared for use as virucides in the treatment of HIV and AIDS. Thus, 2-bromo-5-fluoronitrobenzene was cyclized with CH2:CHMgBr to give 4-fluoro-7-bromoindole, which was treated with ClCOCO2Et, followed by ester hydrolysis to give 4-fluoro-7-bromo-3-indoleglyoxylic acid. This acid was amidated with N-benzoylpiperazine and treated with PhSnBu3 to give I [A = R5 = Ph, W = piperazino, R1, R3, R4, R6 = H, R2 = F]. This compound gave >98% inhibition of HIV-1 infection in HeLa cells.
IT **389630-94-8P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted indoleoxoacetylpiperazines with antiviral activity against HIV-1)

RN 389630-94-8 CAPLUS

CN 1H-Indole-7-carboxylic acid, 3-[[(2R)-4-benzoyl-2-methyl-1-piperazinyl]oxoacetyl]-2,3-dihydro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/630278

=> log h

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	13.02	344.62

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-1.39	-2.78

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 19:49:18 ON 17 APR 2004